SÃ-lvia Simon Rabasseda

List of Publications by Year
in descending order

44 papers	3,184 citations	331259 21 h-index	276539 41 g-index
44 all docs	44 docs citations	44 times ranked	3663 citing authors

#	Article	IF	Citations
1	How does basis set superposition error change the potential surfaces for hydrogenâ€bonded dimers?. Journal of Chemical Physics, 1996, 105, 11024-11031.	1.2	1,882
2	Electron-pairing analysis from localization and delocalization indices in the framework of the atoms-in-molecules theory. Theoretical Chemistry Accounts, 2002, 108, 214-224.	0.5	175
3	Effect of Basis Set Superposition Error on the Water Dimer Surface Calculated at Hartreeâ^'Fock, MÃllerâ^'Plesset, and Density Functional Theory Levels. Journal of Physical Chemistry A, 1999, 103, 1640-1643.	1.1	128
4	Interplay between Intramolecular Resonance-Assisted Hydrogen Bonding and Aromaticity in o-Hydroxyaryl Aldehydes. Journal of Organic Chemistry, 2006, 71, 5241-5248.	1.7	110
5	On the electron-pair nature of the hydrogen bond in the framework of the atoms in molecules theory. Chemical Physics Letters, 2003, 369, 248-255.	1.2	74
6	Interplay between Intramolecular Resonance-Assisted Hydrogen Bonding and Local Aromaticity. II. 1,3-Dihydroxyaryl-2-aldehydes. Journal of Organic Chemistry, 2009, 74, 2059-2066.	1.7	68
7	Structure and fragmentation of glycine, alanine, serine and cysteine radical cations. A theoretical study. Computational and Theoretical Chemistry, 2005, 727, 191-197.	1.5	63
8	Effect of Counterpoise Correction on the Geometries and Vibrational Frequencies of Hydrogen Bonded Systems. Journal of Physical Chemistry A, 2001, 105, 4359-4364.	1.1	57
9	Câ€“Hâ‹¯O H-bonded complexes: How does basis set superposition error change their potential-energy surfaces?. Journal of Chemical Physics, 2000, 113, 5666-5674.	1.2	51
10	The Role of Aromaticity, Hybridization, Electrostatics, and Covalency in Resonance-Assisted Hydrogen Bonds of Adenine-Thymine (AT) Base Pairs and Their Mimics. ChemistryOpen, 2015, 4, 318-327.	0.9	50
11	Isomerization versus Fragmentation of Glycine Radical Cation in Gas Phase. Journal of Physical Chemistry A, 2002, 106, 5697-5702.	1.1	49
12	The proton transfer reaction in malonaldehyde derivatives: Substituent effects and quasi-aromaticity of the proton bridge. Chemical Physics, 2007, 342, 43-54.	0.9	43
13	Influence of the Side Chain in the Structure and Fragmentation of Amino Acids Radical Cations. Journal of Chemical Theory and Computation, 2007, 3, 2210-2220.	2.3	41
14	Dihydrogen Bonding: Donorâ€“Acceptor Bonding (AHâ‹…â‹…â‹…HX) versus the H₂ Molecule (Aï£¿H₂ï£¿X). Chemistry - A European Journal, 2009, 15, 5814-5822.	1.7	32
15	Electron Density Topological Properties Are Useful To Assess the Difference between Hydrogen and Dihydrogen Complexes. Journal of Physical Chemistry A, 2007, 111, 4506-4512.	1.1	29
16	Tuning the Strength of the Resonance-Assisted Hydrogen Bond in o-Hydroxybenzaldehyde by Substitution in the Aromatic Ring¹. Journal of Physical Chemistry A, 2018, 122, 2279-2287.	1.1	28
17	Analysis of the changes on the potential energy surface of Menshutkin reactions induced by external perturbations. Computational and Theoretical Chemistry, 1996, 371, 171-183.	1.5	26
18	Water-catalyzed isomerization of the glycine radical cation. From hydrogen-atom transfer to proton-transport catalysis. Theoretical Chemistry Accounts, 2004, 111, 217-222.	0.5	26

#	ARTICLE	IF	CITATIONS
19	Counterpoise-corrected potential energy surfaces for dihydrogen bonded systems. Chemical Physics Letters, 2004, 386, 373-376.	1.2	24
20	Delocalization indices for non-covalent interaction: Hydrogen and DiHydrogen bond. Computational and Theoretical Chemistry, 2012, 998, 113-119.	1.1	24
21	MHâ‹…sHX Dihydrogen Bond with Mâ‰¡Li, Na and Xâ‰¡F, Cl, Br: A CP-Corrected PES Calculation and an AIM Analysis. Structural Chemistry, 2005, 16, 257-263.	1.0	22
22	Electron transfer from aromatic amino acids to guanine and adenine radical cations in Ï€ stacked and T-shaped complexes. Organic and Biomolecular Chemistry, 2010, 8, 1870.	1.5	22
23	From glycerol to chlorohydrin esters using a solvent-free system. Microwave irradiation versus conventional heating. Tetrahedron, 2009, 65, 10370-10376.	1.0	17
24	Effect of support hydrophobicity of halloysiteâ€based catalysts on the polyalphaolefin hydrofinishing performance. Applied Organometallic Chemistry, 2022, 36, .	1.7	16
25	How the site of ionisation influences side-chain fragmentation in histidine radical cation. Chemical Physics Letters, 2008, 451, 276-281.	1.2	14
26	Towards mild conditions by predictive catalysis via sterics in the Ru-catalyzed hydrogenation of thioesters. Molecular Catalysis, 2021, 510, 111692.	1.0	14
27	Tuning the Strength of the Resonance-Assisted Hydrogen Bond in Acenes and Phenacenes with Two ‹i›o‹/i›-Hydroxyaldehyde Groupsâ€"The Importance of Topology. Journal of Organic Chemistry, 2019, 84, 15538-15548.	1.7	13
28	Experimental and DFT study on titanium-based half-sandwich metallocene catalysts and their application for production of 1-hexene from ethylene. Molecular Catalysis, 2021, 509, 111636.	1.0	12
29	A Fuzzy-Atom Analysis of Electron Delocalization on Hydrogen Bonds. Journal of Physical Chemistry A, 2014, 118, 1142-1149.	1.1	10
30	Gas-phase proton-transport self-catalysed isomerisation of glutamine radical cation: The important role of the side-chain. Theoretical Chemistry Accounts, 2007, 118, 589-595.	0.5	9
31	Excess charge delocalization in organic and biological molecules: some theoretical notions. Theoretical Chemistry Accounts, 2009, 123, 29-40.	0.5	9
32	The impact of the euro crisis on Switzerland. Intereconomics, 2012, 47, 112-119.	1.1	7
33	Conformational dependence of the electronic coupling for hole transfer between adenine and tryptophan. Computational and Theoretical Chemistry, 2011, 975, 38-41.	1.1	6
34	Resonance-Assisted Hydrogen Bondâ€"Revisiting the Original Concept in the Context of Its Criticism in the Literature. International Journal of Molecular Sciences, 2022, 23, 233.	1.8	6
35	Chelation enforcing a dual gold configuration in the catalytic hydroxyphenoxylation of alkynes. Applied Organometallic Chemistry, 2021, 35, e6362.	1.7	5
36	MS-CASPT2 Study of Hole Transfer in Guanineâ€"Indole Complexes Using the Generalized Mullikenâ€"Hush Method: Effective Two-State Treatment. Journal of Physical Chemistry B, 2012, 116, 7815-7820.	1.2	4

#	ARTICLE	IF	CITATIONS
37	On the performance of the Kohnâ€“Sham orbital approach in the calculation of electron transfer parameters. The three state model. Physical Chemistry Chemical Physics, 2014, 16, 17154-17162.	1.3	4
38	Dealing with Quasi-Ring Formation by Two Hydrogen Bonds. Cooperativity Analysis with Delocalization Indices. Journal of Physical Chemistry A, 2014, 118, 9727-9733.	1.1	4
39	Combining Both Acceptorless Dehydrogenation and Borrowing Hydrogen Mechanisms in One System as Described by DFT Calculations. Advanced Theory and Simulations, 0, , 2100566.	1.3	4
40	Electrostatic Interactions Based upon Floating Basis ab Initio Calculations. The Water Pentamer. Journal of Physical Chemistry A, 1997, 101, 1549-1554.	1.1	3
41	Conformational dependence of the electronic coupling in guanineâ€“tryptophan complexes: A DFT study. International Journal of Quantum Chemistry, 2012, 112, 1838-1843.	1.0	2
42	Unveiling the complexity of the dual gold(I) catalyzed intermolecular hydroamination of alkynes leading to vinylazoles. Molecular Catalysis, 2022, 518, 112090.	1.0	1
43	52 GAMES WITH THE PERIODIC TABLE AND BEYOND. , 2019, , .		0
44	GIRONAâ€™S CHEMICAL ITINERARY: 14 YEARS AND A PANDEMIC. INTED Proceedings, 2022, , .	0.0	0